4-Aminoazobenzene 0-09-3 | DTXSID6024460

60-	-09-3	DTXSID602446	6

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 123 °C

Global applicability domain: Inside

Local applicability domain index: 5.11e-01

Confidence level: 6.63e-01

Nearest Neighbors from the Training Set

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4-Aminoazobenzene Measured: 127 Predicted: 123

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Diazoaminobenzene Measured: 98.0 Predicted: 106

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2-(2H-Benzotriazol-2-yl)-4methylphenol

Measured: 132 Predicted: 145

Image not found

1-(Phenylazo)-2-naphthylamine

Measured: 103 Predicted: 113

Image not found

C.I. Solvent Yellow 6
Measured: 126
Predicted: 119